

Fig. 3

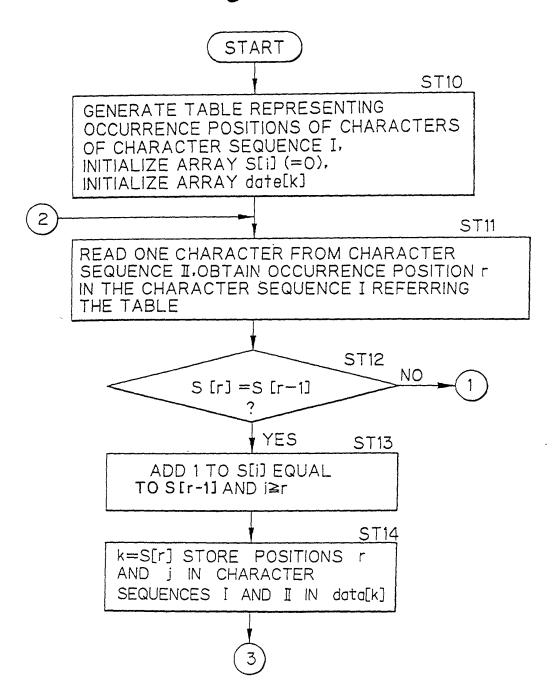


Fig. 4

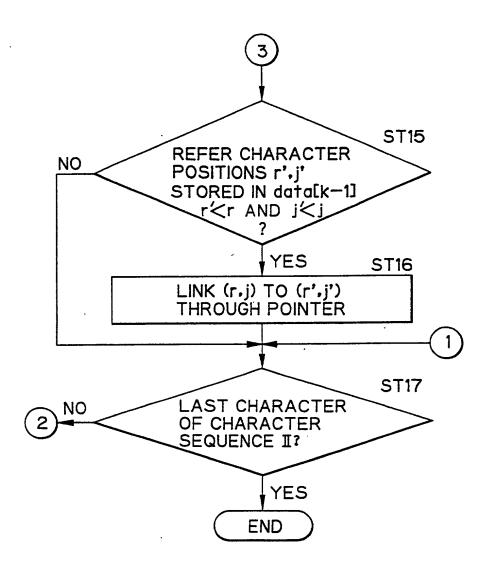
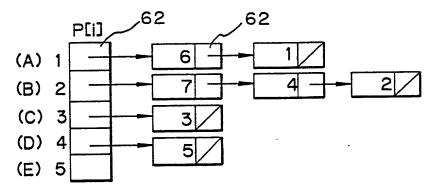


Fig. 5

CHARACTER SEQUENCE I="ABCBDAB"



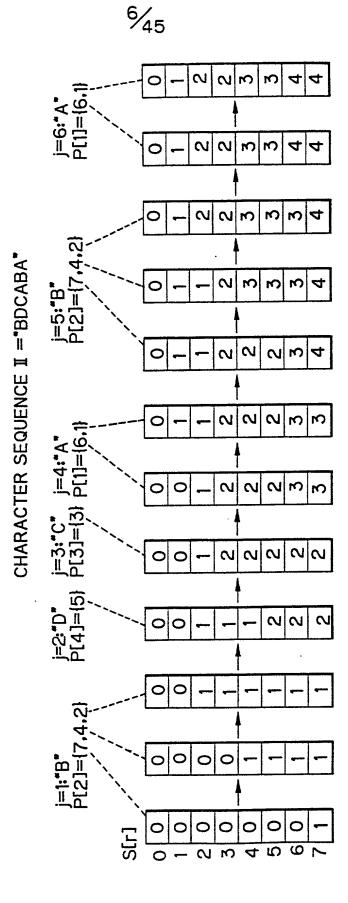


Fig. 6

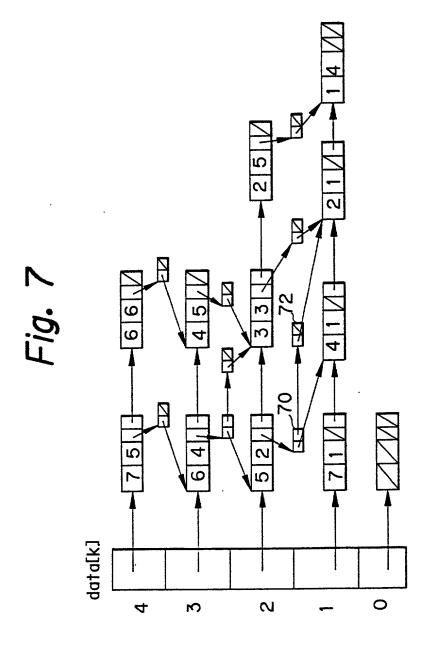


Fig. 8

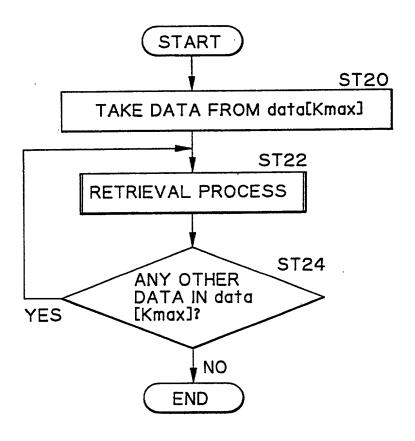
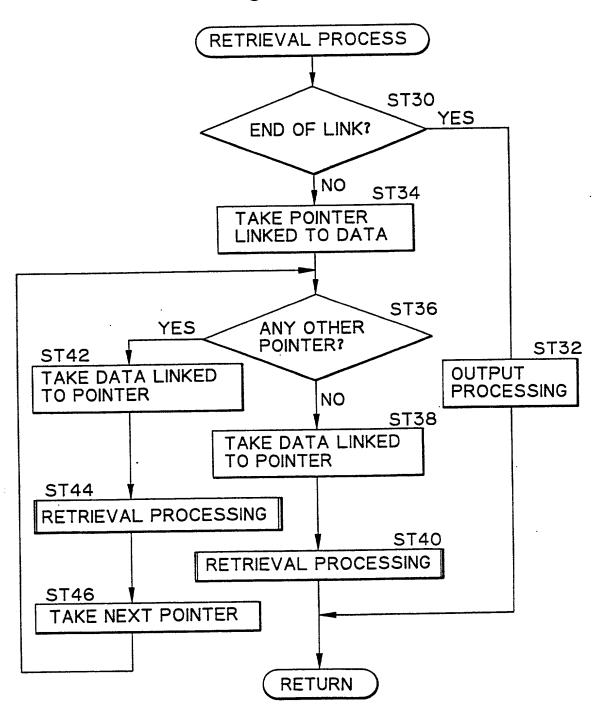


Fig. 9



uman : GDVEKGKKIFIMKCSQCHTVEGGKHKTGPNLHGLFGRK

bacterium : EGDAAAGEKVSKKCLACHTFDQGGANKVGPNPNLFGVF

: GD(x3.3)G(x0.1)K(x0.2)K(x4.0)KC(x2.2)CHT(x3.3)GG(x2.2)K GD(x1.4)E(x0.2)K(x0.2)K(x0.4)KC(x2.2)CHT(x3.3)GG(x2.2)K

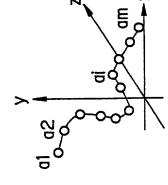
LCS

homology:47%

Rat : MSLAILRVIRLVRVFRIFKLSRHSKGLQILGRTLKASMRELGLLIFFIGVV

(eucinzip, L{6}L{6}L{6}L{6}L

human : GDVEK G K KIFIMKCSQCHTVEKGG KHKTGPNLHGLFGRK... bacterium : E GDAAAGEKVSK KCLACHTFDQGGANKV GPNPN LFGVF...



A={a1,a2,...ai....am}

B={b1.b2....bj....bn}

Fig. 13 D





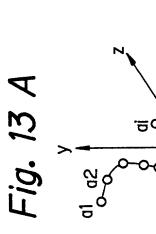
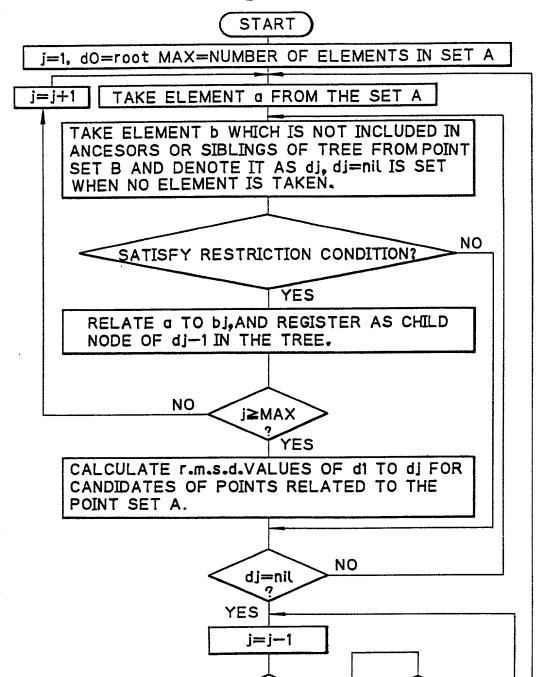


Fig. 13 B

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Fig. 15



NO

j=0

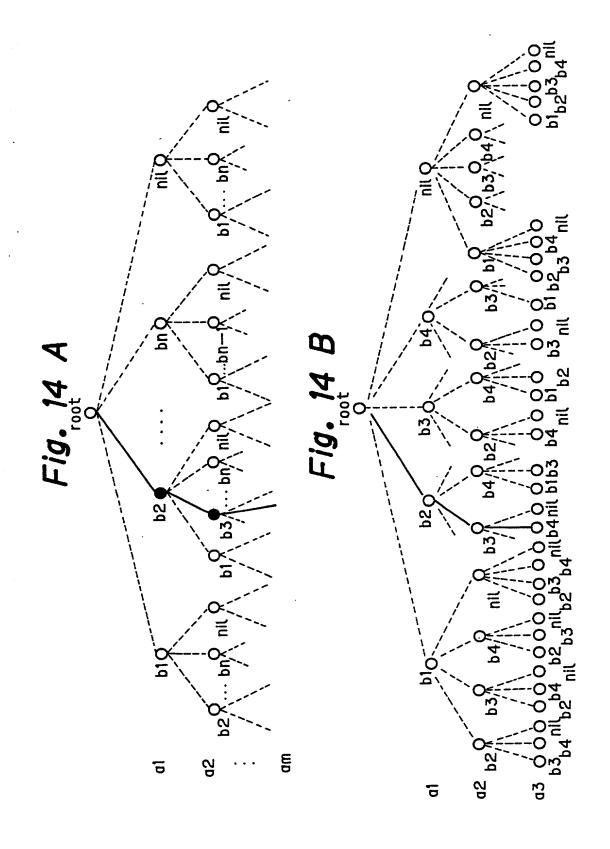
YES

dj=nil

NO

YES

END



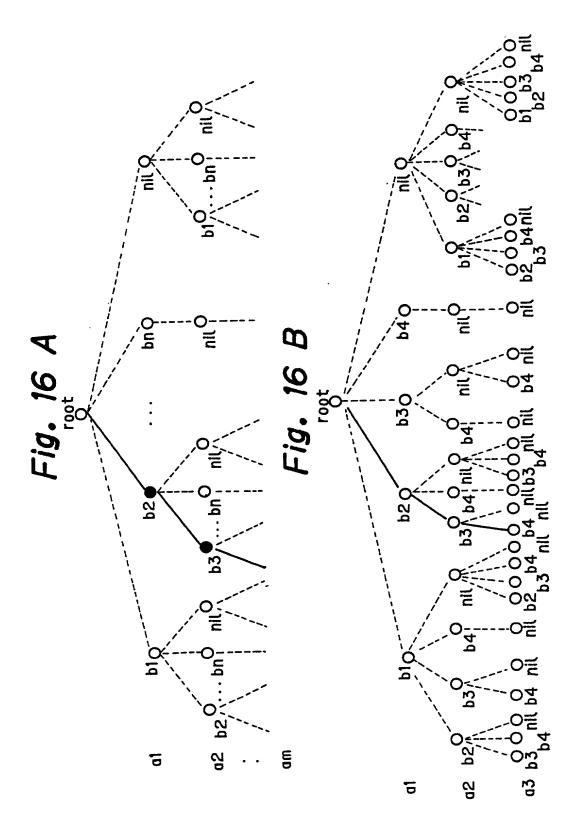
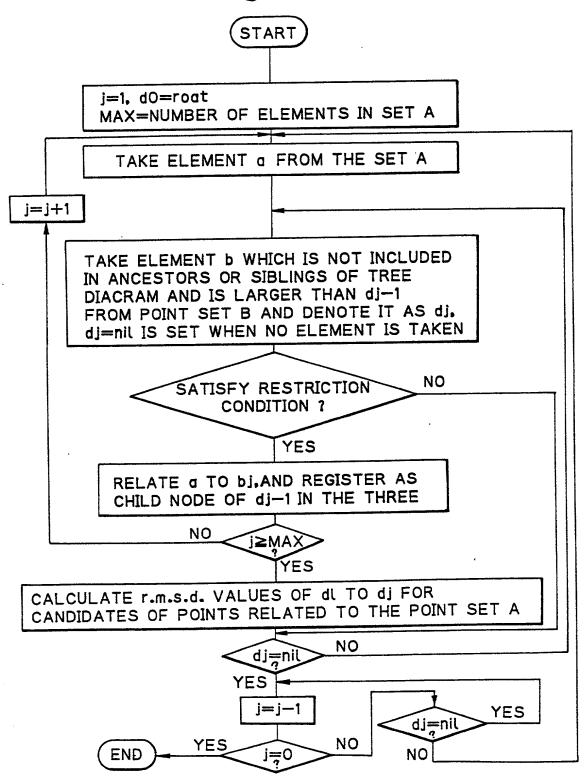
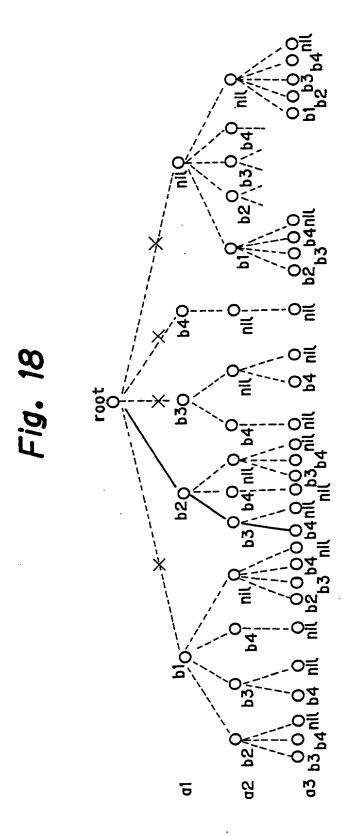


Fig. 17





L G

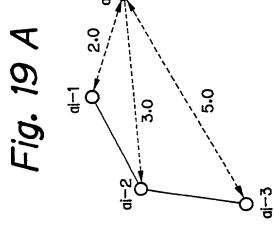


Fig. 20 A

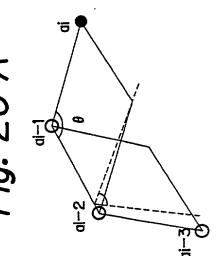
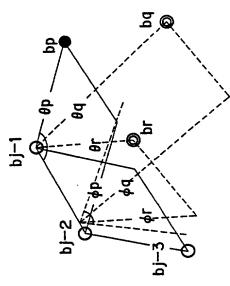


Fig. 20 B



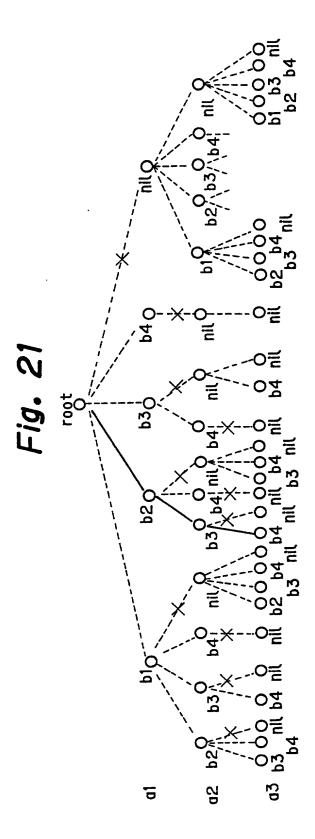


Fig. 22

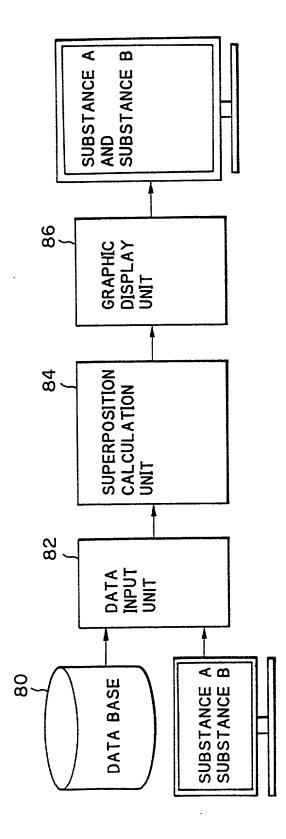


Fig. 23 A

```
TEEQIAEFKE
                AFSLFDKDGD
  GTITTKELGT
                VMRSLGQNPT
21
  EAELQDMINE
                VDADGNGTID
  FPEFLTMMAR
                KMKDTDSEEE
  IREAFRVFDK
                DGNGYISAAE
81
                KLTDEEVDEM
101 LRHVMTNLGE
                QVNYEEFVQM
   IREANIDGDG
121
  MTA
141
```

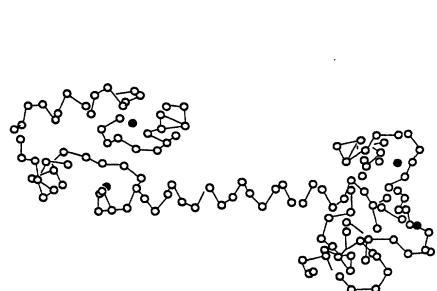
AMINO ACID SEQUENCE OF CALMODULIN (EXCERPT FROM PDB)

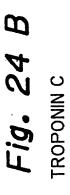
Fig. 23 B

1	AMD'Q Q A E A R A	FLSEEMIAEF
21	KAAFDMFDAD	GGGDISTKEL
41	GTVMRMLGQN	PTKEELDAII
61	EEVDEDGSGT	IDFEEFLVM
81	VRQMKEDAKG	KSEEELADCF
101	RIFDKNADGF	IDIEELGEIL
121	RATGEHVTEE	DIEDLMKDSD
141	KNNDGRIDFD	EFLKMMEGVQ
161	•	

AMINO ACID SEQUENCE OF TROPONIN C (EXCERPT FROM PDB)

Fig. 24 A CALMODULIN





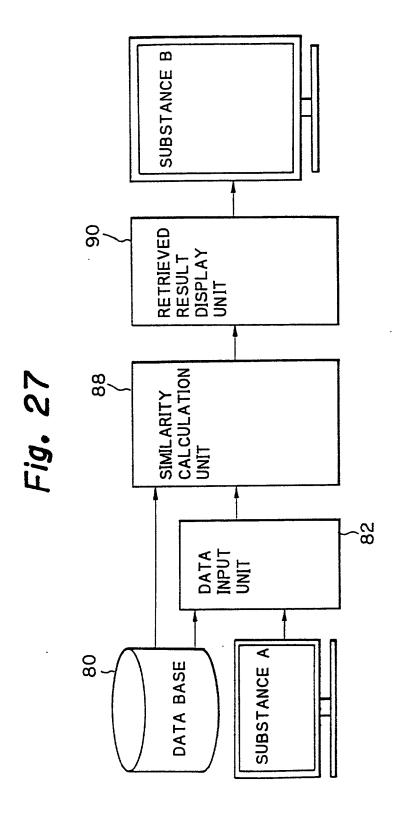


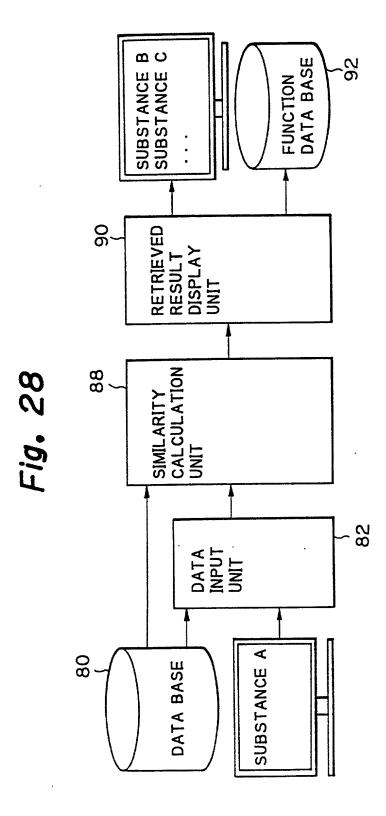




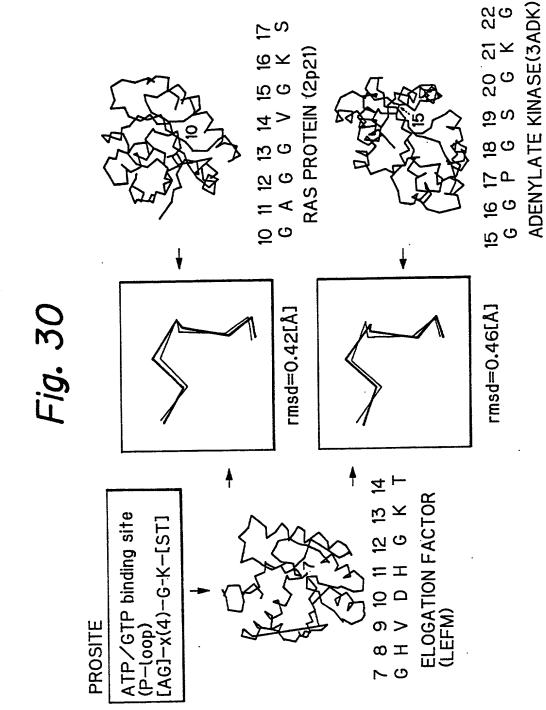
```
< target
                                                                     < probe
                                                                                                           < target >
                                                                                                                              < probe
                                 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110
Probe site = 81-108 in Calmodulin
                                                        R R
                                                                                                                                                          rmsd = 0.567034
```

```
probe
                                                                                                                                                   < probe
                                                                                        < target
                                                                                                                                                                               < target
                                                                                                      probe
                                                                                                                                                                                              probe
                                                                                                                                    G
                                                                                                                    145
                                            ட
                            100 101 102 103 104 105 106 107 108 109 110
                                                                                                                   143
Probe site = 81-108 and 117-143 in Calmodulin
                                                                                                                    142
                                                                                                                                                                5
                                                                                                                                                                <u>|</u>49
                            66 86 26 96
                                                                                                                    132
```





```
assessessessesses ATP/GTP binding site
                                                                                                                                                                                                                                                                                                                                                                                                 10 11 12 13 14 15 16 17
G A G G V G K S < target
G H V D H G K T < probe
rmsd=0.421770 ras protein
                                                                                                                                                                              8 9 10 11 12 13 14 15
G A P G S G K G < target >
G H V D H G K T < probe >
rmsd=0.648732 adenylate kinase
                                                                                                                < probe</pre>
                                         Probe = (elongation factor)
                                                                                         7 8 9 10 11 12 13 14
G H V D H G K T
                                                                                                                                                                                                                                                                                 unit - A
```



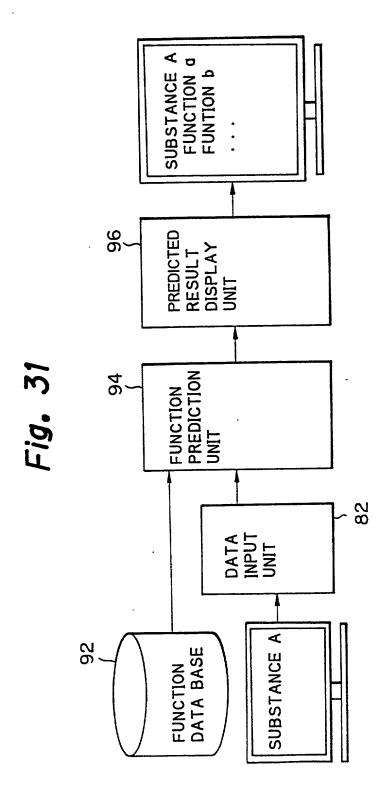


Fig. 32 A Fig. 32 B

LINEAR STRUCTURE NON-LINEAR STRUCTURE

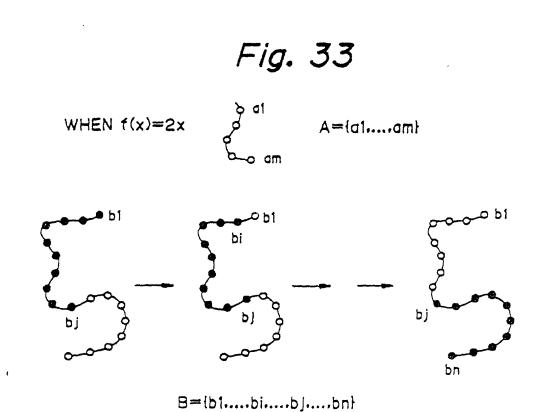


Fig. 34

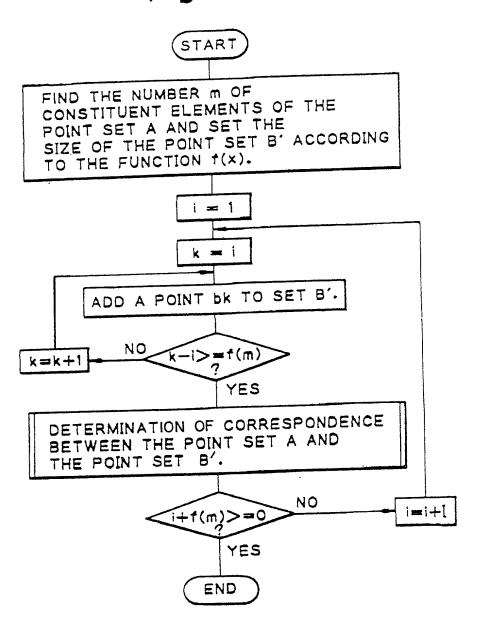
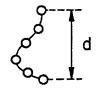
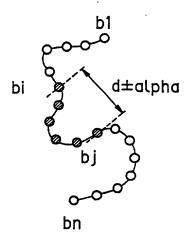


Fig. 35 A



A={a1.a2....am}

Fig. 35 B



B={b1,....bi,....bj,....bn}

START

PREPARE TABLE OF DISTANCE AMONG POINTS OF THE POINT SETS A,B.

FIND DISTANCE BETWEEN TWO POINTS AT BOTH ENDS OF POINT SET A FROM DISTANCE TABLE AND DENOTE IT AS d.

i = 1

j>i bj-bi=d±alpha m<=j-i<=2m

SELECT THE ONE HAVING MAXIMUM J OUT OF dj THAT SATISFY THE ABOVE CONDITIONS.

 $B' = \{bi, bi+1, \cdots bj-1, bj\}$

DETERMINATION OF CORRESPONDENCE BETWEEN POINT SET A AND POINT SET B'

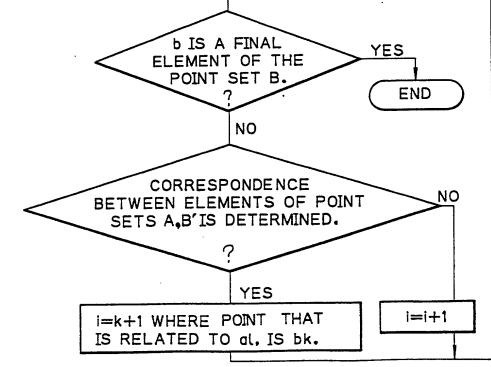


Fig. 37

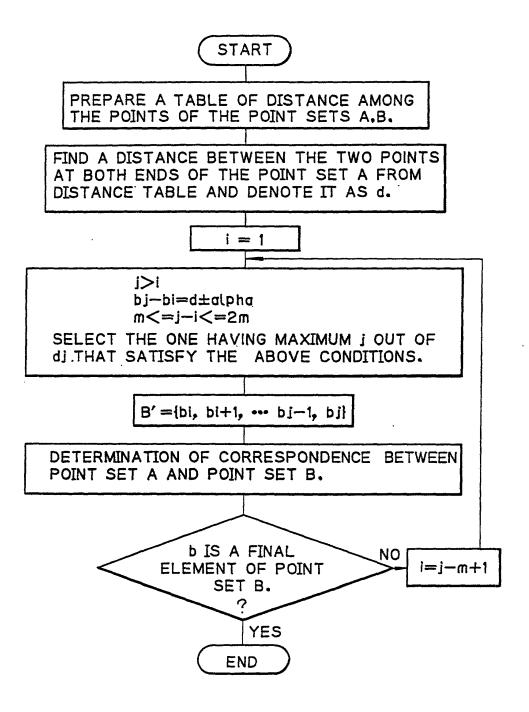


Fig. 38 A

```
TVPYQVSLNS
    VGGYTCCAN
                   NSQWVVS
   GYHFCG
           GSLI
21
          IQVRL
                   GED
    YKS
        G
41
        ISASKS
                   IVHPS
61
                   KSAA
                         S L
   LNND
        IML
81
       SLPTSCA
                   SAG
                       TQC
      I
   A S
101
       TKSSGTS
                           C
                   YPD
   WGN
121
       SDSSCKS
                   AYP
                       G Q
    Ι
141
   FCAGYLEGGK
                         G
                   DSCQ
                          D
161
                   VSWGSGCAQK
       SGKLQGI
   V V C
181
                   NYVSWIKQTI
   NKPGVYTKVC
201
   ASN
221
```

AMINO ACID SEQUENCE OF TRYPSIN (EXCERPT FROM PDB)

Fig. 38 B

```
SWPSQISLQY
   V V G G
         T
          WAHTC
                     GGTL
                           IRQNWV
       SS
   RSG
21
                     LTFR
            VDRE
                              ٧
   MTAAHC
41
                     YVG
              TEQ
     LNQNN
            G
61
                     GYD
                         I
81
   PYWNTDD
                           PR
                      G
                       V L
        T
            S
101
            Y
                     GWGL
     ANSPC
121
                     PTVD
                          YA
      QTL
           Q
            Q
              AYL
141
                     SMVC
                            G
              VKN
      YWG
           S
            T
   S
     S
161
                     PLHC
                            VNGQY
   RSGC
         QGD
              S
               GG
181
   AVHGVTSFVS
                     R L
                        G C
                          NV
                              T
                               RKP
201
   TVFTRVSAYI
                     SWINNV
                              IASN
221
```

AMINO ACID SEQUENCE OF ELASTASE (EXCERPT FROM PDB)

Fig. 39 A

```
Key site number 36 — 41 in Trypsin

41 42 43 44 45 46

M T A A H C \langle trypsin

d = 12.070038 [A]

r.m.s.d. = 0.061077 [A]

The number of atoms in a probe = 6

The number of atoms in PDB = 240

The number of combination = 1

Time = 1sec
```

RETRIEVED RESULTS OF HISTIDINE ACTIVE SITES

Fig. 39 B

```
Key site number 175 - 179 in Trypsin
186 187 188 189 190
                   G
                      < target >
              G
          S
  G
      D
                      < probe</pre>
                   G
      D
  G
d = 8.922721 [A]
r.m.s.d. = 0.092879 [A]
The number of atoms in a probe = 5
The number of atoms in PDB = 240
The number of combination = 1
Time = 1sec
```

RETRIEVED RESULTS OF SERINE ACTIVE SITES

Fig. 40

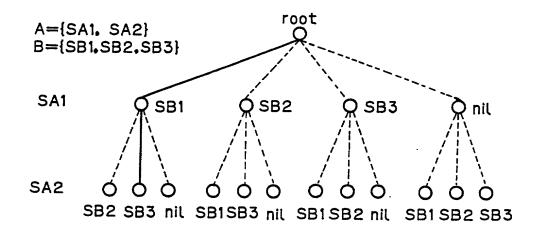
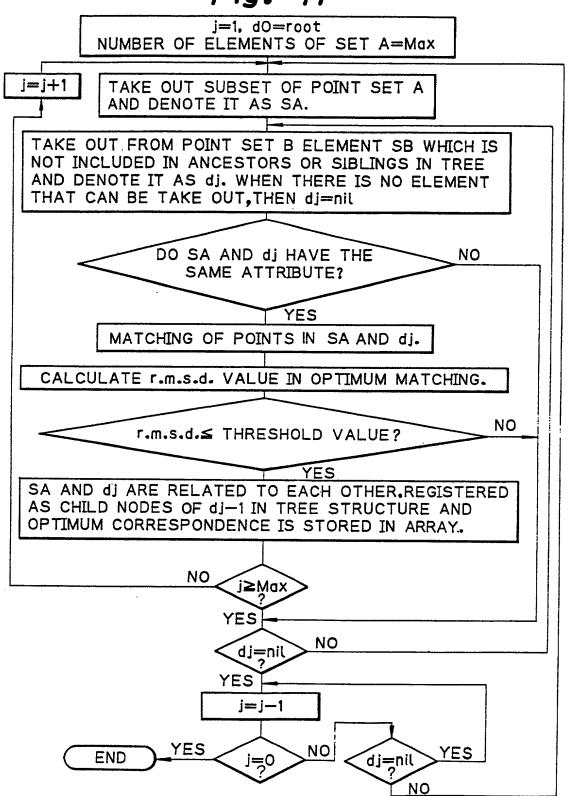
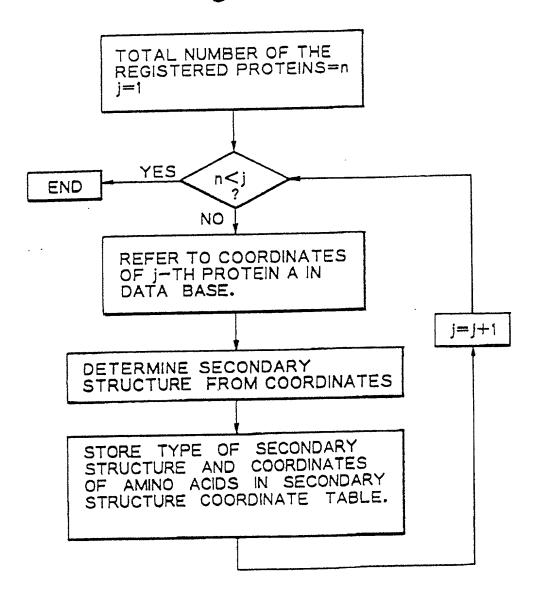


Fig. 41



SECONDARY STRUCTURE COORDINATE TABLE 165 - DISPLAY UNIT 164 162 RETRIEVING UNIT Fig. 42 163 INPUT UNIT SECONDARY STRUCTURE CALCULATION UNIT 161 160 DATA BASE

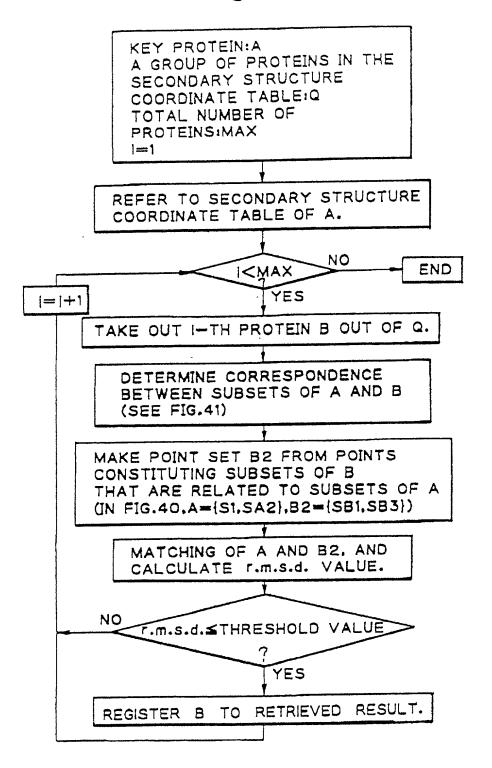
Fig. 43



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SUBSET	COORDINATES	TYPE
S1	{X1,X2,X3,X4,·····Xa}	α - HELIX
S2	{X _{a+1} ,X _{a+2} ,Xb}	α - HELIX
S3	{Xb+1,Xb+2,Xc}	β - SHEET
S4	{Xc+1,Xc+2,Xd}	β — SHEET :
Sn	; {X ₁₊₁ ,X ₁₊₂ ,Xm}	: 3 — TURN

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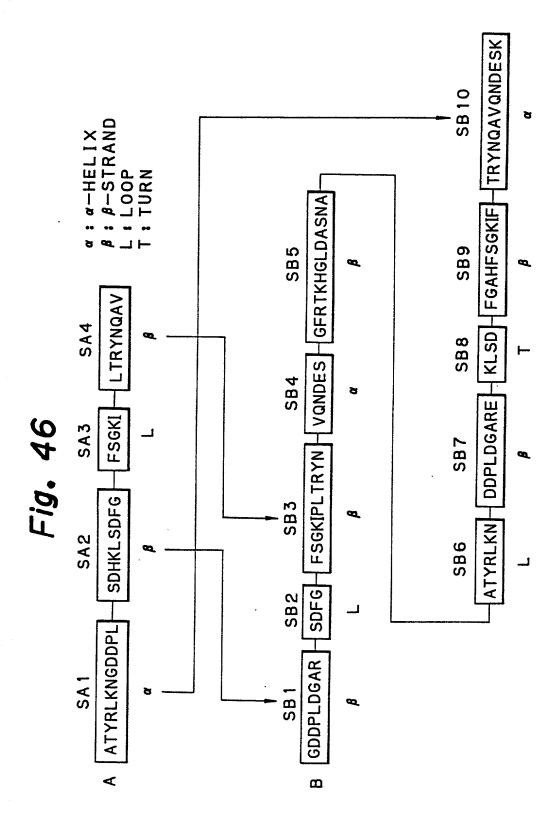
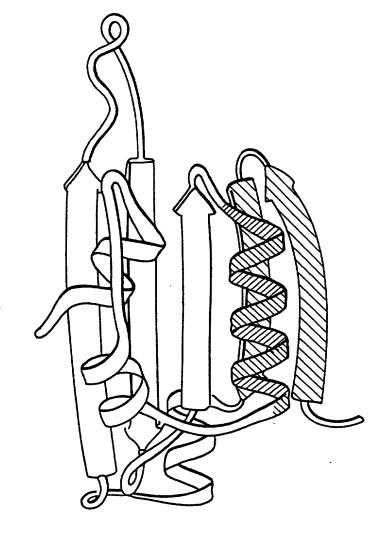


Fig. 47 A

Fig. 47 B



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PROTEIN B HAVING A SIMILAR STRUCTURE

KEY PROTEIN A